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ring nodes :
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ring bonds :
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   19-20 19-24 20-21 21-22 22-23 23-24
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   1-2 1-6 2-3 2-7 3-4 4-5 5-6 5-9
exact bonds :
   6-21
        7-14
normalized bonds :
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19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom

=> s 11

SAMPLE SEARCH INITIATED 18:45:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 76 TO ITERATE

100.0% PROCESSED 76 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 997 TO 2043

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s ll sss full

FULL SEARCH INITIATED 18:46:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2053 TO ITERATE

100.0% PROCESSED 2053 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1

=> d 13 1-4

ANSWER 1 OF 4 REGISTRY COPYRIGHT 2002 ACS L3

457601-25-1 REGISTRY RN

3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)-, dihydrate CN (9CI) (CA INDEX NAME)

OTHER NAMES:

1-(3-Carboxy-2-pyridyl)-4-methyl-2-phenylpiperazine dihydrate C17 H19 N3 O2 . 2 H2 O

MF

SR

CA, CAPLUS, CASREACT, USPATFULL LC STN Files:

CRN (61338-13-4)

●2 H₂O

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2002 ACS
RN 343626-55-1 REGISTRY
CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)-, potassium salt (9CI) (CA INDEX NAME)
MF C17 H19 N3 O2 . K
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
CRN (61338-13-4)

K

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2002 ACS

RN 125967-25-1 REGISTRY

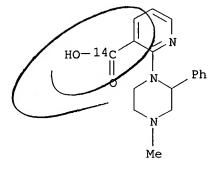
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FS 3D CONCORD

MF C17 H19 N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2002 ACS

RN 61338-13-4 REGISTRY

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-(3-Carboxy-2-pyridyl)-4-methyl-2-phenylpiperazine

FS 3D CONCORD

MF C17 H19 N3 O2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL

(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1962 TO DATE)

6 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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'CSN' IS NOT A VALID FIELD CODE

LEFT TRUNCATION IGNORED FOR '?HYDRATE?' FOR FILE 'REGISTRY'

0 HYDRATE?/CSN

L4 0 L3 AND ?HYDRATE?/CSN

Left truncation is not valid in the specified search field in the specified file. The term has been searched without left truncation. Examples: '?TERPEN?' would be searched as 'TERPEN?' and '?FLAVONOID' would be searched as 'FLAVONOID.'

If you are searching in a field that uses implied proximity, and you used a truncation symbol after a punctuation mark, the system may interpret the truncation symbol as being at the beginning of a term. Implied proximity is used in search fields indexed as single words, for example, the Basic Index.

=> help field codes
HELP FOR 'FIELD CODES' IS NOT AVAILABLE
For information about help messages available in all files, enter
"HELP MESSAGES". For information about help messages available for
the current file, enter "HELP DIRECTORY". For a list of commands,
enter "HELP COMMANDS".

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 148.12 148.33

FULL ESTIMATED COST

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FILE COVERS 1907 - 17 Dec 2002 VOL 137 ISS 25 FILE LAST UPDATED: 16 Dec 2002 (20021216/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 13

L5 7 L3

=> d 15 1-7 bib abs hitstr

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L5
     ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS
AN
     2002:695977 CAPLUS
DN
     137:216962
TI
     Methods for the preparation of mirtazapine intermediates
IN
     Metzger, Leonid; Wizel, Shlomit
PA
     Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals USA,
so
     PCT Int. Appl., 12 pp.
     CODEN: PIXXD2
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DT
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LΑ
     English
FAN.CNT 1
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                             DATE
                                             APPLICATION NO.
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
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             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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PRAI US 2001-272699P
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                             20010301
OS
     CASREACT 137:216962
AB
     The prepn. of 1-(3-carboxy-2-pyridy1)-4-methyl-2-phenylpiperazine
     dihydrate (I) and other mirtazapine intermediates are described. These
     compds. are particularly useful in the prepn. of mirtazapine. Thus,
     1-(3-cyano-2-pyridy1)-4-methyl-2-phenylpiperazine was hydrolyzed with aq.
     KOH, neutralized with HCl and the ppt. washed with water to give I whose
     crystal structure is reported.
     457601-25-1P, 1-(3-Carboxy-2-pyridyl)-4-methyl-2-phenylpiperazine
IT
     dihydrate
     RL: IMF (Industrial manufacture); PRP (Properties); RCT (Reactant); SPN
     (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
        (prepn. of 1-(3-carboxy-2-pyridyl)-4-methyl-2-phenylpiperazine
        dihydrate as an intermediate for mirtazapine)
RN
     457601-25-1 CAPLUS
CN
     3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)-, dihydrate
           (CA INDEX NAME)
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2 H₂O

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5
     ANSWER 2 OF 7 CAPLUS COPYRIGHT 2002 ACS
AN
     2002:368461 CAPLUS
DN
     136:369741
TI
     A novel method for preparation of piperazine and its derivatives
IN
     Sebastian, Sonny; Patel, Hetal Virendra; Thennati, Rajamannar
PA
     Sun Pharmaceutical Industries Ltd., India
SO
     PCT Int. Appl., 23 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
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                        KIND
                                                APPLICATION NO.
                               DATE
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              HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
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     BE 1013317
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                               20001107
     WO 2001-IN129
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     CASREACT 136:369741; MARPAT 136:369741
OS
GΙ
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AB Compds. I [R = H, C1-6 alkyl, phenyl-C1-4 alkyl; R1 = H, Me,(un) substituted phenyl; R2 = H, Me, fluoromethyl] useful as starting materials for prepn. of pharmaceutically active compds. are prepd. by reacting R1COCO2R with H2NCH2CHR2NHR to give 3,4-dehydropiperazine-2-one and its derivs., followed by reacting with a reducing agent to yield I. Thus, 1-methyl-3-phenylpiperazine was prepd. and used as starting material for prepn. of 1,2,3,4,10,14b-hexahydro-2-methyl-pyrazino[2,1-a]pyrido[2,3c}[2]benzazepine. IT

61338-13-4P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of piperazine derivs. as starting materials for prepn. of pharmaceutically active compds.)

RN 61338-13-4 CAPLUS

3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) CN

INDEX NAME)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS
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     2001:435071 CAPLUS
AN
DN
     135:33494
     Process for the preparation of a pyridinemethanol compound
TI
IN
     Iishi, Eiichi; Yoshikawa, Kanami
PA
     Sumika Fine Chemicals Co., Ltd., Japan
SO
     PCT Int. Appl., 30 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     Japanese
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     WO 2001042240
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     WO 2000-JP6688
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     CASREACT 135:33494
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GI
       CO-OK
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AB A pyridinemethanol compd. useful as an important intermediate for the prepn. of mirtazapine effective as an antidepressant can be prepd. by reducing a potassium salt of pyridinecarboxylic acid as represented by formula I with a metal hydride. Thus, 1-butanol 162, KOH 60.93, and

Me

2-(4-methyl-2-phenylpiperazin-1-yl)pyridine-3-carbonitrile oxalate 40 g were heated to give potassium 2-(4-methyl-2-phenylpiperazin-1-yl)pyridine-3-carboxylate, which was reduced in THF with 12.5 g lithium aluminum hydride to give 21.78 g 2-(4-methyl-2-phenylpiperazin-1-yl)pyridine-3-methanol (yield 70.78%).

IT 343626-55-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of pyridinemethanol compd. as intermediate for mirtazapine)

RN 343626-55-1 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)-, potassium salt (9CI) (CA INDEX NAME)

K

IT 61338-13-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of pyridinemethanol compd. as intermediate for mirtazapine)

RN 61338-13-4 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS
L5
AN
     2001:435070 CAPLUS
DN
     135:33493
ΤI
     Process for the preparation of a pyridinemethanol compound
IN
     Iishi, Eiichi; Yoshikawa, Kanami
PA
     Sumika Fine Chemicals Co., Ltd., Japan
SO
     PCT Int. Appl., 30 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     Japanese
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               `Me
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AB A pyridinemethanol compd. serving as an important intermediate of mirtazapine useful as antidepressant can be prepd. by reducing a potassium salt of a pyridinecarboxylic acid as represented by formula I with a metal hydride.

IT 343626-55-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of pyridinemethanol compd. as intermediate for mirtazapine)

RN 343626-55-1 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)-, potassium salt (9CI) (CA INDEX NAME)

● K

IT 61338-13-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of pyridinemethanol compd. as intermediate for mirtazapine)

RN 61338-13-4 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5
     ANSWER 5 OF 7 CAPLUS COPYRIGHT 2002 ACS
AN
     2000:756528 CAPLUS
DN
     133:321900
TI
     Novel synthesis and crystallization of piperazine ring-containing
     compounds such as mirtazapine
IN
     Singer, Claude; Liberman, Anita; Finkelstein, Nina
PA
     Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals Usa,
SO
     PCT Int. Appl., 22 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
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GΙ
```

AB Mirtazapine, useful in treating depression (no data), was prepd. by reacting pyridine I [R1 = CH2OH, CH2Cl, CH2Br, CH2I; R2 = NH2] with compd. II [R3 = Cl, F, Br, I] followed by treating the resulting piperazine III with H2SO4. The mirtazapine intermediate 1-(3-carboxypyridly-2)-4-methyl-2-phenylpiperazine may be made by hydrolyzing 1-(3-cyanopyridyl-2)-4-methyl-2-phenylpiperazine with KOH at a temp. of at least about 130.degree.C. The present invention also relates to new processes for recrystn. of mirtazapine form crude mirtazapine.

IT 61338-13-4P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (novel synthesis and crystn. of piperazine ring-contg. compds. such as mirtazapine)

RN 61338-13-4 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2002 ACS

AN 1990:139001 CAPLUS

DN 112:139001

TI The synthesis of Org 3778 labeled with tritium, carbon-13 and carbon-14

AU Kaspersen, Frans M., Van Rooij, Fons A. M.; Sperling, Eric G. M.; Wieringa, Joop H.

CS Sci. Dev. Group, Organon Int. BV, Oss, 5340 BH, Neth.

SO Journal of Labelled Compounds and Radiopharmaceuticals (1989), 27(9), 1055-68

CODEN: JLCRD4; ISSN: 0362-4803

DT Journal

LA English

OS CASREACT 112:139001

GΙ

AB The syntheses of 1,2,3,4,10,14b-hexahydro-2-methylpyrazino[2,1-a]pyrido[2,3-c][2]benzazepine (Org 3770, I) labeled with 3H (and 2H), 13C and 14C are described. Tritiated I was prepd. either by exchange under alk. conditions with tritiated water or catalytic reductive dehalogenation of a chloro analog with 3H2. 13C-labeled material was obtained in a 7-step synthesis starting from 13C-labeled benzene, whereas I-14C was prepd. in a 3-step synthesis starting with 14CO2.

IT 125967-25-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and redn. of)

Ι

RN 125967-25-1 CAPLUS

CN 3-Pyridinecarboxylic-14C acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2002 ACS

AN 1977:29883 CAPLUS

DN 86:29883

TI Heterocyclic tetracyclic compounds

IN Van der Burg, Willem J.

PA AKZO N. V., Neth.

SO Ger. Offen., 40 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.		KIND	DATE	APPLICATION NO.		DATE
ΡI	DE	2614406	A1	19761014	DE	1976-2614406	19760402
	DE	2614406	C2	19920220			
	NL	7504075	Α	19761007	NL	1975-4075	19750405
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	NL	189199	С	19930201			
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PRAI		1975-4075		19750405			
	NL	1975-75040		19750405			
GI							

AB The title compds., e.g. I and II, with nervous system-depressant and antihistaminic activities (no data), are prepd. by various procedures. Thus, reaction of 2-chloronicotinonitrile with 1-methyl-3-phenylpiperazine gives 2-(4-methyl-2-phenyl-1-piperazinyl)-3-pyridinecarbonitrile which is

hydrolyzed to the carboxylic acid which is reduced to the hydroxymethyl deriv. (III). Cyclization of 3.25 g III in concd. $\tt H2SO4$ at 20-35.degree. gives after 2 hr and treatment with NH4OH 2.43 g I.

IT 61338-13-4P

RN 61338-13-4 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-(4-methyl-2-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

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